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Determination of the minimum island size for full exciton localization due to thickness fluctuations in $Zn_{1-x}Cd_xSe$ quantum wells

P. Diaz-Arencibia and I. Hernandez-Calderon
Physics Department, CINVESTAV, Apdo. Postal 14-740, 07000 Mexico, D.F. Mexico

Abstract. Atomic layer fluctuations of the thickness of quantum wells (QWs) are one of the causes of exciton localization. Here, we present the results of the determination of the minimum lateral dimensions of islands formed by thickness fluctuations in $Zn_{1-x}Cd_xSe$ QWs which produce full exciton localization. We have calculated the localization energy of excitons in the frame of the factorized-envelope approximation. We found that the excitons are well localized in the islands of the QW when their dimensions are larger than ~15 times the exciton Bohr radius. This result allows us to evaluate the quality of the QW structure and interpret the photoluminescence characteristics of QWs.

Introduction

In ideal QW structures the interfaces are flat planes, free of imperfections. However, in real QWs the interfaces present structural and chemical defects that result in potential fluctuations which alter the motion of the particles within the QW. In high quality QWs these defects result in flat, large area regions of constant thickness, these large regions (that we will call terraces) present differences in thickness of one or two monomolecular layers (ML, 1 ML $= a/2$, where a is the lattice constant). Then, for the case of a high quality QW structure with average thickness $Na/2$, where N is the number of ML, it is normally expected the existence of terraces $(N \pm 1)a/2$ and $(N \pm 2)a/2$ thick and in such a way that QW thickness fluctuations will give place to exciton localization [1]. Since the 1s energy of the exciton localized in an $(N + 1)$-terrace will be lower than the 1s energy of an exciton localized at an N-terrace, at low temperatures and low excitation levels the $(N + 1)$-QWs will be the most populated; $U \equiv E_{1s}(N) - E_{1s}(N + 1)$ is the barrier height that localizes the exciton inside the $(N + 1)$-QW; $E_{1s}(N)$ is the energy of the free 1s exciton in the N-monolayer thick QW. As the temperature raises, the assistance of acoustical phonons makes possible the migration of excitons to the N-terraces. For this process to occur the exciton must overcome the localization energy $\Delta E \leq U$. ΔE may be lower than U when the QW has regions with reduced lateral dimensions L_x, L_y in such a way that confinement effects caused by the comparable spatial extensions of the $(N + 1)$-thick *island* and the wavefunction of the exciton result in the raising of the ground state of the 1s exciton and then a lowering of the localization energy. In other words, additional quantization in the x and y directions (z is perpendicular to the QW plane) reduces the energy that the exciton needs to migrate to the N-thick terrace. Many of the phenomena related to exciton localization and phonon assisted migration can be observed when studying the photoluminescence (PL) vs. temperature characteristics of high quality QWs. The analysis requires a clear identification of the different excitonic emission mechanisms which may be present in the QW PL spectrum [2]. Bound excitons (BX) [3] and biexcitons (BB) [4, 5] have been assigned to optical transitions in the PL spectra of $Zn_{1-x}Cd_xSe$ QWs. In previous papers we have analyzed in detail the mechanisms of exciton localization and exciton migration as a function of temperature for the case of two structurally different $Zn_{1-x}Cd_xSe$ QWs grown by molecular beam epitaxy (MBE) with different barrier materials [2, 6, 7]. Based on those studies we have made estimates of the relative total area of islands with different thickness, but that analysis does not give information about the area of individual islands [2]. In the following we will present a calculation of the minimum size (L_x, L_y) of an $(N+1)$ island that is necessary to produce *full* localization of excitons, that is, when $\Delta E \approx U = E_{1s}(N) - E_{1s}(N+1)$.

1. Theory

The minimum size of an $(N+1)$-island with full exciton localization can be estimated calculating the 1s energy of the exciton as a function of their lateral dimensions. The $(N+1)$-island is assumed to be laterally surrounded by a N thick QW and is formed in one of the interfaces while the opposite interface is completely flat. The islands are assumed to have a rectangular shape $L_x \times L_y$ and the energy of the barrier that localizes the exciton in the $(N+1)$-island is U. The calculations are made using the factorized-envelope approximation described by Gupalov, Ivchenko and Kavokin [8] and references therein. In the case of very large islands or islands with square shape, the 1s state is doubly degenerated, however, the islands will generally be asymmetric, breaking this degeneracy. Then, the ground state of the localized exciton will be denoted by $E_{1s}^{xy}(N+1)$. We solve the Schrödinger equation for the in-plane envelope function of the exciton $F(X,Y)$, which describes the localization of the 1s exciton as a whole within the island, where X and Y are the components of the in-plane exciton center of mass radius vector $R_\parallel \equiv (X,Y)$ of the localized exciton at the island. If we represent $F(X,Y)$ as a product of separate functions $F_X(X)$ and $F_Y(Y)$, the Schrödinger equation is decomposed in a set of two coupled Hartree equations:

$$\begin{cases} \left[-\frac{\hbar}{2M}\frac{\partial^2}{\partial X^2} - UP_Y\theta\left(\frac{L_x}{2} - |X|\right)\right]\cdot F_X(X) = -\varepsilon_X F_X(X) \\ \left[-\frac{\hbar}{2M}\frac{\partial^2}{\partial Y^2} - UP_X\theta\left(\frac{L_y}{2} - |Y|\right)\right]\cdot F_Y(Y) = -\varepsilon_Y F_Y(Y) \end{cases} \tag{1}$$

Here θ is the step function; $\theta(s \geq 0) = 1, \theta(s < 0) = 0$. The energies ε_X and ε_Y determine the localization energy $\Delta E = \varepsilon_X + \varepsilon_Y - U \cdot P_X \cdot P_Y$; where P_X and P_Y are the coupling factors of Eqs. (1) and are just the particle probability density inside the island:

$$P_X = \int_{-L_x/2}^{L_x/2} F_X^2(X)\mathrm{d}X \quad \text{and} \quad P_Y = \int_{-L_y/2}^{L_y/2} F_Y^2(Y)\mathrm{d}Y \tag{2}$$

P_X, $P_Y < 1$ since the functions $F_X(X)$ and $F_Y(Y)$ extend beyond the potential barriers of the island. The localization energy can be also written as $\Delta E = E_{1s}(N) - E_{1s}^{xy}(N+1)$. The boundary conditions demand that the envelope functions $F_X(X)$, $F_Y(Y)$ and their derivatives in the directions perpendicular to the sides of the rectangle are continuous on the perimeter of the island.

2. Results and discussion

Calculations were made for two structurally different $Zn_{1-x}Cd_xSe$ QWs [2, 6, 7]. The parameters used in calculation are listed in Table 1.

The results are shown in Fig. 1, the exciton localization energy ΔE is plotted as a function of the dimensions of the island. Each curve represents an island with constant L_y

Table 1. Parameters used in calculations; $M_w = m_e^w + m_{hh}^w$ and $M_B = m_e^B + m_{hh}^B$.

Sample	x	L_w (Å)	E_g (eV)	M_w/m_0	M_B/m_0	U (meV)
A-809	0.69	40	2.028	0.582	0.63	11.7
C-161	0.26	50	2.482	0.612	0.63	8.8

and varying L_x, in terms of integer multiples of the exciton Bohr radius a_B. As can be seen, the localization energy ΔE of the fundamental state $E_{1s}^{x,y}$ approaches U when the dimensions of the sides L_x and L_y of the rectangular island are of the order or larger than 15 times the exciton Bohr radius, i.e, larger than ~600 Å. This means that the minimum area of the $(N+1)$ island for a full exciton localization is of the order of 3.08×10^{-3} μm^2 and 4.36×10^{-3} μm^2 for samples A-809 and C161, respectively. When one of the sides of the rectangle is less than $15a_B$ the exciton localization energy is less than U. This means that the exciton is not fully localized in the island. The presence of small $(N+1)$-islands ($L_x, L_y < 15a_B$) will lead to contributions in the emission spectrum of the QW at intermediate energies compared to those corresponding to the N-QW and $(N+1)$-islands with $L_x, L_y > 15a_B$. The excitation energy ΔE that the exciton needs to migrate at higher temperatures is then also less than U. The conclusion is that it is necessary for the islands to present dimensions in L_x and L_y much larger than the Bohr radius in order to achieve full localization of excitons. Then, as a consequence, a careful examination of the PL spectrum of a QW can give substantial information about its structural quality, the energy of the emission peaks and their spectral width are directly related to the abundance and size of the islands produced by thickness fluctuations of the QW. Moreover, the PL bands could be not symmetric. Broadening of the PL spectra at the high energy side of the $(N+1)$-QW

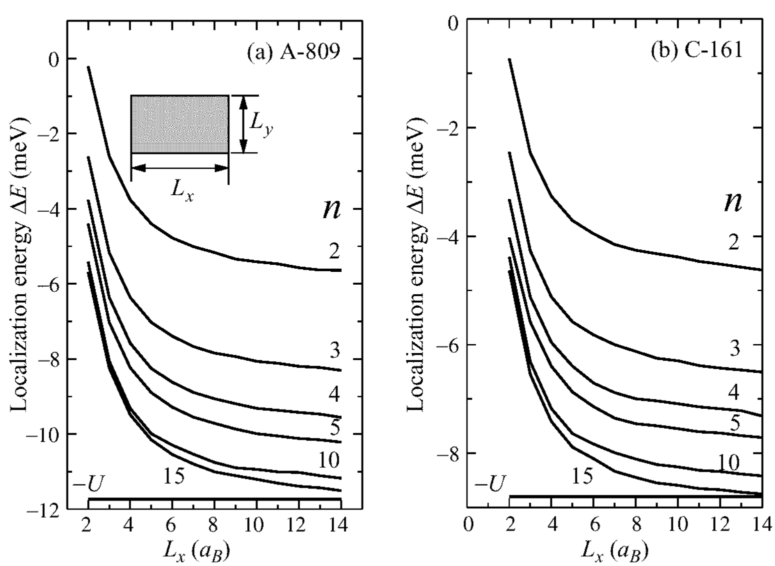

Fig. 1. Localization energy of the fundamental state of excitons localized at $(N+1)$ and $(N+2)$-islands for samples A-809 and C-161, respectively. (a) Sample A-809 $N+1 = 14$, $U = 11.7$ meV. (b) Sample C-161, $N+2 = 19$, $U = 8.8$ meV.

and in the low energy side of the N-QW may appear due to inhomogeneous broadening caused by the size distribution of the $(N+1)$-islands. Examination under this criteria of the PL spectra of the emission of QWs A-809 and C161 allows us to conclude that the main emission peaks correspond to islands with full localization, therefore having lateral dimensions of at least 15 times the Bohr radius of the exciton. The fact that two (symmetric) gaussian lines fit very well the PL emission suggests that those QWs are formed by large terraces, as expected in high quality QWs.

In summary, in the frame of the factorized-envelope approximation we have obtained the localization energy of excitons in II–VI QWs as a function of the lateral dimensions of a $(N+1)$-island within a N-QW. We found that for a full exciton localization ($\Delta E \sim U$) the lateral sizes of the island (L_x, L_y) must be larger than $\sim$15 times the exciton Bohr radius, i.e, L_x, $L_y \gg a_B$. This analysis helps to the interpretation of the excitonic features in the PL spectra and brings information useful to the evaluation of the structural properties of QWs.

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